



Los Alamos National Laboratory brings next-generation HPC to the fight against COVID-19

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LOS ALAMOS, N.M., Oct. 20, 2020—Los Alamos National Laboratory has completed the installation of a next-generation high performance computing platform, with aim to enhance its ongoing R&D efforts in support of the nation's response to COVID-19. Named Chicoma, the new platform is poised to demonstrate Hewlett Packard Enterprise's new HPE Cray EX supercomputer architecture for solving complex scientific problems.

"As extensive social and economic impacts from COVID-19 continue to grip the nation, Los Alamos scientists are actively engaged in a number of critical research efforts ranging from therapeutics design to epidemiological modeling," said Irene Qualters, Associate Laboratory Director for Simulation and Computing at Los Alamos. "High Performance Computing is playing a critical role by allowing scientists to model the complex phenomena involved in viral evolution and propagation."

Chicoma is among the earliest deployments of the HPE Cray EX supercomputer, which offers a large-scale system architecture with a next-generation system software stack, direct-to-chip liquid cooling capabilities and a newly designed HPE Slingshot interconnect. It features the AMD EPYC™ 7H12 processor and in total, more than 73,000 cores, and 300 TB of system memory. These new capabilities are at the forefront of technologies anticipated for the DOE's Office of Science and National Nuclear Security Administration multi-lab Exascale Computing Initiative, and will provide scientists with substantially higher supercomputing performance than is currently available in other Los Alamos National Laboratory systems.

"Los Alamos National Laboratory has been working closely with researchers through the COVID-19 HPC Computing Consortium as well as with local researchers to harness the power of the Lab's HPC compute capabilities to stop the spread of COVID-19. This newest HPC asset will be a significant addition to that endeavor," said Qualters.

This new HPC system at Los Alamos will be quickly put to task on a range of COVID-19 research problems. Foremost of these will be epidemiological modeling of contact patterns and intervention scenarios, bioinformatics studies of SARS-CoV-2 gene development, and impacts of COVID-19 on human 3D chromosome structure and function.

"The Chicoma system will be an ideal platform for our high performance computing efforts in chromosome simulation, RNA simulation including viruses, and chromosome-

virus effects,” said Dr. Karissa Sanbonmatsu, senior scientist in the Laboratory’s Theoretical Biology and Biophysics group.

Chicoma’s enhanced capability for COVID-19 research was funded by the Department of Energy’s Office of Science Advanced Scientific Computing Research (ASCR) program, under a line item of the 2020 Coronavirus Aid, Relief, and Economic Security (CARES) Act.

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